



chain nodes :

7	8	9	19	20	27	28	42	43
74	75	76	80	83	90	97	98	

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15 16 17 18 21 22 23 24 25 26 29 30 31 32
33 34 35 36 37 38 39 40 41 45 46 47 48 49 50 51 52 53 54 55 56 57 58 82

chain bonds :

3-9 4-8 6-7 16-20 18-19 24-28 26-27 30-43 31-42 32-97 41-44 43-62 46-60 47-59
 48-80 49-98 58-61 60-73 62-63 62-64 64-65 65-66 66-67 66-90 70-71 75-76 82-83

ring bonds :

1-6	1-2	2-3	3-4	4-5	5-6	10-11	10-12	11-13	12-14	13-14	13-15	14-18	15-16	16-17
17-18	21-26	21-22	22-23	23-24	24-25	25-26	29-30	29-32	30-31	31-82	32-82	33-34		
33-35	34-36	35-37	36-37	36-38	37-41	38-39	39-40	40-41	45-46	45-49	46-47	47-48		
48-49	50-51	50-52	51-53	52-54	53-54	53-55	54-58	55-56	56-57	57-58				

exact/norm bonds :

exact bonds :

3-9 30-43 43-62 46-60 60-73 70-71 75-76

normalized bonds :

36-37 36-38 37-41 38-39 39-40 40-41 53-54 53-55 54-58 55-56 56-57 57-58

G1: [*1], [*2]

G2: [*3], [*4], [*5], [*6], [*7]

G3 : [*8], [*9], [*10], [*11], [*12]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS 21:Atom
22:Atom

23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS 29:Atom 30:Atom 31:Atom
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom
42:CLASS 43:CLASS 44:CLASS 45:Atom 46:Atom 47:Atom 48:Atom 49:Atom 50:Atom 51:Atom
52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:CLASS 60:CLASS 61:CLASS
62:CLASS 63:CLASS 64:CLASS 65:CLASS 66:CLASS 67:CLASS 68:CLASS 69:CLASS 70:CLASS
71:CLASS 72:CLASS 73:CLASS 74:CLASS 75:CLASS 76:CLASS 80:Atom 82:Atom 83:Atom 90:CLASS
97:CLASS 98:CLASS